

Collisionless hydrodynamics for 1D motion of inhomogeneous degenerate electron gases: equivalence of two recent descriptions

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Abstract

Recently I. Tokatly and O. Pankratov ("TP", Phys. Rev. B 60, 15550 (1999)) used velocity moments of a classical kinetic equation to derive a hydrodynamic description of electron motion in a degenerate electron gas. Independently, the present authors (Theochem 501-502, 327 (2000)) used considerations arising from the Harmonic Potential Theorem (Phys. Rev. Lett. 73, 2244 (1994)) to generate a new form of high-frequency hydrodynamics for inhomogeneous degenerate electron gases (HPT-N3 hydrodynamics). We show here that TP hydrodynamics yields HPT-N3 hydrodynamics when linearized about a Thomas-Fermi groundstate with one-dimensional spatial inhomogeneity.

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I. INTRODUCTION

The prediction of collective oscillations in degenerate electron gases is a very old problem that has been addressed over the years at many different levels of theory. In the limit of an infinite *homogeneous* electron gas it has been possible to apply relatively sophisticated microscopic theory beyond the Random Phase (RPA) approximation^{1,2}. The main current issue in the degenerate case of the uniform gas is the effect of electron-electron correlations on the relevant response functions, leading to modified dispersion relations at finite wavenumber, possibly presaging quantum phase transitions. Interestingly, however, the homogeneous plasmons both in two and three dimensions are completely determined by sum rules in the zero-wavenumber limit, so that elementary hydrodynamic arguments give the correct answers in this limit.

The situation is not so well advanced for *inhomogeneous* degenerate electron gases, where high-level dynamic microscopic theory is unwieldy, though the RPA has been carried through some time ago for simple-metal surface geometries³. Calculations of the RPA type are now possible at the numerical level for molecules and possibly larger systems via a number of quantum-chemistry-inspired packages. Some form of Time Dependent Density Functional Theory can include the correlation physics approximately^{4,5}. All of these microscopic approaches are rather computationally intensive, however.

In order to deal with long-wavelength response in a computationally simple fashion, Bloch⁶ and others very long ago introduced a hydrodynamic style of treatment for degenerate electron systems. Various workers^{7,8,9,10,11}, have used this idea in linearized form with the assumption that the pressure perturbation is proportional to the density perturbation. In the early treatments, inhomogeneity of the gas was envisaged only in terms of edges bounding an otherwise uniform gas, and these edges were treated via postulated boundary conditions. Such approaches, often with a “hard-wall” boundary condition¹⁰, have given a largely reasonable description of collective plasmon modes in confined systems such as thin metal slabs and quantum wells, with however some shortcomings to be discussed below. Be-

cause plasmons are high-frequency phenomena, the connection between pressure and density perturbations in a gas of uniform density n ,

$$\delta p = m\beta^2\delta n \quad (1)$$

had to be used with a nonstandard "high-frequency" value of the coefficient β derivable from microscopic Lindhard response theory, namely

$$\beta^2 = \frac{3}{5}v_F^2(n) = \frac{3}{5}\hbar^2(3\pi^2n)^{2/3}/m^2 \quad (2)$$

instead of the low-frequency value

$$\beta^2 = \frac{1}{3}v_F^2(n) \quad (3)$$

derivable from the static pressure-density relation for a degenerate electron gas.

An obvious defect of the hydrodynamic approach is that it can be guaranteed only to describe the "classical" size effects such as standing plasmons in which a finite number of nodes of the electron density perturbation fit across the thin dimension of an electron gas layer. By contrast, "quantum" size effects involve details of wavefunctions and are not necessarily given by hydrodynamic theory: these size effects are related directly to transitions between discrete quantum states due to spatial confinement of the electrons. These two categories of mode are not fully distinct, however¹²: for example, the sloshing or Kohn mode of the electron gas in a parabolic quantum well can be regarded either as due to transitions between two Harmonic Oscillator states, or as an odd combination of surface plasmons¹³. Nevertheless, it is clear that in general there can be many more modes in a microscopic treatment than in the corresponding hydrodynamic one.

Apart from the lack of the complete spectrum of quantum size-effect modes, the hydrodynamic approach, as usually applied, has other drawbacks for confined electron gases. Firstly, it has mostly been used under the assumption that the electron gas is spatially homogeneous. This assumption then requires a separate treatment of edge effects, via somewhat arbitrary boundary conditions at the edge of the uniform-gas region. For example, the

hard-wall boundary conditions and uniform spatial profile frequently used to analyze plasmons on charge-neutral electron gases of finite width¹⁰ give a reasonable description of the 2D plasmon and sloshing modes (equivalent to even and odd combinations of surface plasmons) but not the multipole surface plasmons, which require a selvage of finite width. For an electron gas under parabolic confinement (non-neutral gas) on the other hand, the same hard-wall condition does not seem to be so appropriate^{14,15}, and “free” boundary conditions have been suggested along with some further assumptions..

The hydrodynamic approach is particularly tricky for plasmon modes that are intrinsically tied to inhomogeneity, such as the multipole surface plasmons of a neutral jellium surface. These modes depend intimately on the detailed decay of the electron density at the edge, and this cannot be treated by a simple, single boundary condition on a uniform gas. There have been attempts within hydrodynamics to model the edge by a series of steps, each with its own distinct but internally homogeneous density¹⁶, in which case additional boundary conditions must be used. Hydrodynamic models have also been investigated with a smoother but somewhat arbitrary surface density profile^{7,17,18}. The problem then is that the profile is not internally generated, and in some of these approaches the pressure term was not properly consistent with the chosen inhomogeneous density profile.

In connection with inhomogeneous or bounded degenerate gases, we have taken the point of view^{19,20} that hydrodynamics should be applied to a continuously varying model of edges (or of inhomogeneity in general). In addition, one should use a smooth solution of the groundstate problem that is consistent with the hydrodynamic approximation chosen. Then arbitrary boundary conditions can be kept to a minimum or removed altogether. In addition, the pressure term should be properly adapted to the inhomogeneity. For plasmon applications on a finite slab of electron gas, we tried the obvious inhomogeneous generalization of the high-frequency Bloch approach by using a high-frequency inhomogeneous pressure coefficient (2) $\beta^2(n_0(\vec{r})) = \frac{3}{5}v_F^2(n_0(\vec{r}))$, where $n_0(\vec{r})$ is the selfconsistent Thomas-Fermi groundstate density profile. This approach was found¹⁹, however, to violate the Harmonic Potential Theorem (HPT). This theorem is an extension of the Generalized Kohn Theorem²¹

and states among other things that, for systems confined by a harmonic external potential (e.g. the electron gas in a parabolic quantum well), there exists a plasmon mode in which the inhomogeneous groundstate density (and groundstate many-body wavefunction) oscillates rigidly at the bare harmonic oscillator frequency. This violation was subsequently²² discussed in a more general fashion, from the viewpoint of invariance under transformation to an accelerated reference frame²³. In Eqs. (21)-(24) of the original HPT paper¹⁹ a modification of collisionless Bloch hydrodynamics was suggested in order to satisfy the HPT. That version of hydrodynamics was later found to violate Newton's third law (momentum conservation), but this was rectified to produce a theory that we here term the HPT-N3 hydrodynamics²⁰. HPT-N3 theory was applied successfully²⁰ to describe both the Kohn and standing-plasmon modes of a parabolic quantum well gas. We have also been able²⁴ to use HPT-N3 hydrodynamics to see multipole surface plasmons at the surface of a near-neutral electron gas, without using additional boundary conditions.

It is this modified HPT-N3 hydrodynamic theory that will be discussed further here and compared with another hydrodynamic theory. Specifically, Tokatly and Pankratov ("TP") in two recent papers ("TP1"²⁵, "TP2"¹⁵) derived a hydrodynamic theory valid both for low and high frequencies, by taking moments of an assumed semiclassical kinetic equation. They did not, however, explicitly examine the case of spatially inhomogeneous groundstates (other than via assumed boundary conditions on a homogeneous gas). We will show here that this TP theory agrees with the HPT-N3 theory in the collisionless limit, when taken to second order in gradients and linearized about the appropriate Thomas-Fermi groundstate of an electron gas with general one-dimensional inhomogeneity. Since the two derivations of the pressure term are quite different, this agreement tends to support the validity of both theories for the case of 1D inhomogeneity.

The present work is organized as follows. In Section II a brief summary is given of the HPT-N3 theory. In section III the collisionless TP equations through second order are quoted for the simplified case of 1D spatial variations. In Section IV these 1D TP equations are linearized about the inhomogeneous TF groundstate and the result is shown to be precisely

the HPT-N3 theory²⁰. Section V is devoted to discussion and conclusions.

II. SUMMARY OF LINEARIZED HPT-N3 HYDRODYNAMICS

The exact equation of motion (Euler, Newton II) for the fluid velocity $\vec{u}(\vec{r}, t)$ is

$$mn\left(\frac{\partial}{\partial t} + \vec{u} \cdot \vec{\nabla}\right)\vec{u} = -\vec{\nabla} \cdot \mathbf{P} + n\vec{F} \quad (4)$$

where $\mathbf{P}(\vec{r}, t)$ is the stress-pressure tensor (not known exactly in general), $n(\vec{r}, t)$ is the number density, and $\vec{F}(\vec{r}, t)$ is the (external plus internal) force per electron due to interactions, usually treated via some form of mean-field theory. The pressure force per electron, i.e. the force due to streaming of particles from one fluid element into another, is $\vec{F}^{press} = -n^{-1}\vec{\nabla} \cdot \mathbf{P}$. The form (4) guarantees that the net force on the system due to pressure is zero: specifically, the total system pressure force is

$$F^{press, tot} = \int n(\vec{r}, t) \vec{F}^{press}(\vec{r}, t) d\vec{r} = \int (-\vec{\nabla} \cdot \mathbf{P}) d\vec{r} = 0$$

Linearizing (4) about a non-streaming ($\vec{u}_0 = 0$) equilibrium state we obtain

$$mn_0(\vec{r}) \frac{\partial}{\partial t} \vec{u}_1(\vec{r}, t) = -\vec{\nabla} \cdot \mathbf{P}_1(\vec{r}, t) + n_1(\vec{r}, t) \vec{F}_0(\vec{r}) + n_0(\vec{r}) \vec{F}_1(\vec{r}, t) \quad (5)$$

The approach introduced previously¹⁹ in order to accommodate the HPT in a Bloch-style inhomogeneous hydrodynamics was to use the fluid displacement \vec{x} defined by

$$\vec{x}(\vec{r}, t) \equiv \int_{t_0}^t \vec{u}(\vec{r}, t') dt' \quad (6)$$

to write the density perturbation n_1 as the sum of a compressive part n_{1A} and a dispersive part n_{1B} :

$$n_1(\vec{r}, t) = -\vec{\nabla} \cdot (n_0(\vec{r}) \vec{x}(\vec{r}, t)) \quad (7)$$

$$= n_{1A}(\vec{r}, t) + n_{1B}(\vec{r}, t) \quad (8)$$

$$n_{1A}(\vec{r}, t) = -n_0(\vec{r}) \vec{\nabla} \cdot \vec{x}(\vec{r}, t) \quad (9)$$

$$n_{1B}(\vec{r}, t) = -\vec{x}(\vec{r}, t) \cdot \vec{\nabla} n_0(\vec{r}) \quad (10)$$

Equation (7) is exact to linear order and can be obtained from a time integration of the linearized continuity equation (conservation of electrons). Eqs. (8)-(10) are also exact. Note that n_{1B} represents the density perturbation that would result if the groundstate density distribution were locally displaced rigidly without compression, while n_{1A} represents the density perturbation due to compression. For Kohn-mode motion in which the groundstate is translated rigidly, $n_{1B} = n_1$ while $n_{1A} = 0$ because there is no compression. By contrast, for oscillations about a spatially homogeneous equilibrium state for which $\vec{\nabla} n_0 = \vec{0}$, we have $n_{1A} = n_1$ while $n_{1B} = 0$.

Thus in order to satisfy the known Lindhard limit for high-frequency response of a uniform gas, it was proposed¹⁹ that n_{1A} be associated in general with the high-frequency pressure coefficient $\beta^2(\infty) = \frac{3}{5}v_F^2$. Similarly to obtain the correct HPT behavior for inhomogeneous harmonically-confined systems it was further proposed¹⁹ that n_{1B} be associated with the low-frequency coefficient $\beta^2(0) = \frac{1}{3}v_F^2$, because the static groundstate pressure profile must be rigidly translated in Kohn-mode motion. Then the pressure perturbation (assumed^{19,20} to be a scalar rather than the more general tensor) is

$$p_1^{HPTN3}(\vec{r}, t) = mv_F^2(n_0(\vec{r}))[\frac{3}{5}n_{1A}(\vec{r}, t) + \frac{1}{3}n_{1B}(\vec{r}, t)] \quad (11)$$

$$P_{1ij} = \delta_{ij}p_1^{HPTN3} \quad (12)$$

where

$$v_F^2(n_0(\vec{r})) = \hbar^2 m^{-2} (3\pi^2 n_0(\vec{r}))^{2/3} \quad (13)$$

is the square of the local Fermi velocity corresponding to the groundstate number density $n_0(\vec{r})$. Although motivated by the limiting uniform and quadratically-confined cases, Eq. (11) was proposed as a general result.

The linearized HPT-N3 theory is completed by inserting (11)-(13) into the linearized Euler equation (5). For the situations of interest here where all space dependence is in the z direction, this gives

$$0 = mn_0 \partial_t u_1 - \partial_z \left(\frac{3}{5} m v_F^2 n_0 \partial_z \xi + \frac{1}{3} m v_F^2 \xi \partial_z n_0 \right) - n_1 F_0 - n_0 F_1. \quad (14)$$

Here ξ is the fluid displacement in the z direction from (6),

$$\xi(z, t) = \int_{t_0}^t u_1(z, t') dt', \quad (15)$$

and v_F is a position-dependent Fermi velocity determined by the inhomogeneous groundstate density n_0 :

$$v_F^2 = \hbar^2 m^{-2} (3\pi^2 n_0(z))^{2/3}. \quad (16)$$

Equations (14) - (16) are the basic equations of linear HPT-N3 hydrodynamics²⁰ for a degenerate electron gas where both the groundstate and excitations exhibit one-dimensional spatial inhomogeneity. They were derived so as to satisfy the Harmonic Potential Theorem¹⁹ (HPT), to obey conservation of particle number and of momentum (hence Newton III, N3), and to give the correct limit of high-frequency plasma dispersion in a uniform electron gas as in microscopic degenerate response (Lindhard-RPA) theory. We will show elsewhere²⁶ that the HPT-N3 equations can alternatively be derived from nonlinear time dependent density functional theory with a very simple assumption regarding memory. The HPT-N3 equations represent an improvement over the HPT hydrodynamics originally proposed¹⁹, in that the original form did not satisfy Newton III.

We will now outline the Tokatly and Pankratov (TP) hydrodynamic theory^{25,15}, then compare it with the HPT-N3 theory summarized above, for the case of one-dimensional spatial variations and linear perturbations. Despite their very different derivations, these two theories will be shown to agree for this 1D case.

III. THE TP HYDRODYNAMIC MOMENT EQUATIONS FOR ONE-DIMENSIONAL SPATIAL VARIATION

Tokatly and Pankratov^{25,15} obtained hydrodynamic-style equations by taking velocity moments of a classical kinetic equation, assuming that this equation is adequate for degenerate Fermi particles, presumably with a fully degenerate Fermi distribution in mind as the static solution.

They decoupled the set of hydrodynamic moment equations, using the smallness of the parameter

$$\gamma = \frac{\langle p/m \rangle}{L \max\{\omega, \nu_c\}} \quad (17)$$

where $\langle p/m \rangle$ is the average particle speed, $L \equiv q^{-1}$ measures the spatial scale of the hydrodynamic perturbation, and ν_c is an appropriate collision frequency. We are interested in the high-frequency, collisionless case for which $\omega \gg \nu_c$ and collision integrals can be ignored as discussed by TP. To $O(\gamma^2)$, their first three 1D moment equations (Eqs. (16), (17) and (18) of their first paper²⁵) are then, in our notation,

$$\begin{aligned} m\left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial z}\right)n(z, t) + mn\frac{\partial}{\partial z}u &= 0 \\ \therefore \frac{\partial}{\partial t}n + \frac{\partial}{\partial z}(nu) &= 0 \quad (\text{continuity}) \end{aligned} \quad (18)$$

$$\begin{aligned} mn\left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial z}\right)u + \frac{\partial}{\partial z}P - nF &= 0 \\ &(\text{Newton II}) \end{aligned} \quad (19)$$

$$\begin{aligned} \left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial z}\right)P + 3P\frac{\partial}{\partial z}u(z, t) &= 0 \\ &(\text{evolution of stress - pressure}). \end{aligned} \quad (20)$$

Here the number density n , fluid velocity u , the stress-pressure tensor component $P \equiv P_{zz}$, and the total force F due to interactions, are all functions of the single space coordinate z and the time t . (The three-dimensional generalization of (18) - (20) is given by Equations (22) - (25) of TP2¹⁵, with $\mathbf{L}^{(3)}$ and $\mathbf{I}^{(2)}$ set to zero.) Our notation in (18)-(20) is chosen to match that of our recent work²⁰. The connections with the notation of TP1²⁵ are as follows, with our notation on the left:

$$\begin{aligned} z &\rightarrow x, \\ n &= m^{-1}L^{(0)}, \\ u &= v, \end{aligned}$$

$$P = P_{xx} = L^{(2)},$$

$$V = -e\phi,$$

$$F = +e\partial_x\phi.$$

IV. COMPARISON OF LINEARIZED HPT-N3 AND TP THEORIES

In linearizing (18) - (20), Tokatly and Pankratov immediately replaced the convective derivative $D_t \equiv \partial_t + \vec{u} \cdot \vec{\nabla}$ by the partial derivative ∂_t . (See Eqs. (23)-(26) of TP1²⁵ and Eqs.(46) - (49) ff. of TP2¹⁵). In particular, this implies that quantities such as $\partial P_0/\partial z$ and $\partial n_0/\partial z$ are set to zero, where $P_0(z)$ is the equilibrium pressure-stress tensor component and $n_0(z)$ is the groundstate density profile. Thus they specialized to systems with a spatially uniform groundstate, without actually stating this condition. They thereby also removed the possibility of treating edge inhomogeneities other than via assumed boundary conditions. Because of the homogeneous assumption they were furthermore unable to discuss the Harmonic Potential Theorem fully, even though some reference was made to it in Section V of TP2¹⁵. Note that the essential feature of the HPT, which makes it a more stringent test of many-particle theories compared with the Generalized Kohn Theorem²¹ (GKT), is that the entire groundstate many-body wavefunction, and hence all derived quantities such as $n_0(\vec{r})$ and $P_0(\vec{r})$, are rigidly translated in HPT motion, giving $n(\vec{r}, t) = n_0(r - X(t))$, $P(\vec{r}, t) = P_0(r - X(t))$ etc., where the center-of-mass coordinate $X(t)$ satisfies the classical simple-harmonic-oscillator equation of motion. To verify satisfaction of the HPT, it is not sufficient to show that the centre of mass moves appropriately as in TP2¹⁵: the preservation of the inhomogeneous groundstate spatial profiles $n_0(\vec{r})$, $P_0(\vec{r})$ in the moving situation is also an essential feature.

A. Equilibrium state

Fortunately it is easy to linearize (18)-(20) without discarding the space derivatives of groundstate quantities. First note that, for a 3D electron gas in a 1D situation where spatial variation of all quantities occurs only in the z direction, the kinetic equation for the equilibrium distribution function f_0 is

$$\{m^{-1}p_z\partial_z + F_{0z}\frac{\partial}{\partial p_z}\}f_0(z, \vec{p}) = 0 \quad (21)$$

where $\vec{F}_0 = F_{0z}\hat{z}$ is the total selfconsistent force due to interactions. If $F_0(z) = -\partial_z V_0(z)$, then direct substitution into (21) verifies that the equilibrium solutions are of the form

$$f_0(z, \vec{p}) = A\left(\frac{1}{2m}\vec{p}^2 + V_0(z)\right), \quad \vec{p}^2 \equiv p_x^2 + p_y^2 + p_z^2$$

where $A(\varepsilon)$ is an arbitrary function of one variable. For a degenerate electron gas, the classical kinetic theory will optimally describe the quantal situation if A is chosen to be the Fermi distribution

$$A(\varepsilon) = C\theta(\mu - \varepsilon), \quad (22)$$

where C and μ are independent of z and \vec{p} . The groundstate density is then

$$n_0(z) = \int f_0(z, \vec{p}) d^3p = C \int_0^{p_F(z)} 4\pi p^2 dp = C \frac{4\pi}{3} p_F^3(z)$$

where C is a constant and

$$p_F(z) = mv_F(z) = \sqrt{2m(\mu - V_0(z))}.$$

Note that this assumption of a local Fermi distribution with a global chemical potential amounts to a Thomas-Fermi type of theory, which is therefore the natural groundstate theory to accompany a hydrodynamic treatment of excitations in a degenerate system.

The zz component of the stress-pressure tensor from this distribution (see Eqs. (3) and (13) of TP1²⁵)

is

$$\begin{aligned}
P_{0zz} &\equiv L_{0zz} = \frac{1}{m} \int p_z p_z f_0(\vec{r}, \vec{p}) d^3p = \frac{1}{3} \frac{1}{m} \int \vec{p}^2 f_0(z, \vec{p}) d^3p \\
&= \frac{1}{3} \frac{1}{m} \int p^2 C \theta(p_F(z) - p) 4\pi p^2 dp \\
&= \frac{1}{3m} \frac{4\pi}{5} p_F^5(z) = \frac{1}{5m} p_F^2(z) n_0(z) = \frac{m}{5} v_F^2(z) n_0(z) \propto n_0(z)^{5/3}
\end{aligned} \tag{23}$$

Then

$$\partial_z P_{0zz} \equiv \partial_z L_{0zz}^{(2)} = \partial_z n_0 \frac{\partial P_{0zz}}{\partial n_0} = \partial_z n_0 \frac{5}{3} \frac{P_{0zz}}{n_0} = \partial_z n_0 \frac{1}{3m} p_F^2(z) = \partial_z n_0 \frac{m}{3} v_F^2(z) \tag{24}$$

B. Linearized moment equations of TP

Linearizing our Eqs. (18)-(20) about the Thomas-Fermi groundstate just described, we write

$$\begin{aligned}
n(\vec{r}, t) &= n_0(z) + n_1(z, t) \\
u(\vec{r}, t) &= 0 + u_1(z, t) \\
P_{zz}(\vec{r}, t) &= P_{0zz}(z) + P_1(z, t) \\
F(\vec{r}, t) &= F_0(z) + F_1(z, t)
\end{aligned}$$

and obtain

$$\partial_t n_1 + n_0 \frac{\partial u_1}{\partial z} = 0 \tag{25}$$

$$mn_0 \frac{\partial u_1}{\partial t} + \partial_z P_1 - n_0 F_1 - n_1 F_0 = 0 \tag{26}$$

$$\partial_t P_1 + u_1 \partial_z P_{0zz} + 3P_{0zz} \partial_z u_1 = 0 \tag{27}$$

where n_1 , u_1 and P_1 are functions of z and t whereas n_0 , F_0 and P_{0zz} are functions of z alone. Note that the $u_1 \partial_z P_{0zz}$ term in (27) is missing in (e.g.) Eq. (49) of TP2 or Eq. (26) of TP1 because TP have assumed a uniform unperturbed system so that $D_t = \partial_t$. It is

this additional term in our treatment which ensures satisfaction of the true HPT (not just the GKT which is satisfied by the treatment of TP involving uniform gas with zero-stress boundary condition).

Insertion of the equilibrium pressure tensor and its space derivative from (23) and (24) into (27) gives

$$\partial_t P_1 + u_1(\partial_z n_0) \frac{m}{3} v_F^2(z) + \frac{3m}{5} v_F^2(z) n_0 \partial_z u_1 = 0 \quad (28)$$

$$-\partial_t P_1 = \frac{m}{3} v_F^2(z) u_1 \partial_z n_0 + \frac{3m}{5} v_F^2(z) n_0 \partial_z u_1. \quad (29)$$

We integrate both sides with respect to time, up to time t from an initial equilibrium at time t_0 when all perturbations vanished. Then using (15) we obtain

$$P_1 = -\frac{m}{3} v_F^2(z) \xi \partial_z n_0 - \frac{3m}{5} v_F^2(z) n_0 \partial_z \xi. \quad (30)$$

Inserting (30) into (26) we obtain

$$mn_0 \frac{\partial u_1}{\partial t} - \partial_z \left(\frac{m}{3} v_F^2(z) \xi \partial_z n_0 + \frac{3m}{5} v_F^2(z) n_0 \partial_z \xi \right) - n_0 F_1 - n_1 F_0 = 0 \quad (31)$$

Eq. (31) derived from the Tokatly-Pankratov approach²⁵ is identical to Eq. (14) derived from the HPT-N3 theory²⁰. This equivalence is the principal result of the present paper. Eq. (31) has already been shown²⁰ to give a sensible treatment of both the Kohn mode and the hydrodynamic standing plasmon modes of the electron gas in a parabolic quantum well, while taking into account the smooth decay of the electron density at the edges and using only “natural” boundary conditions that the fluid displacement ξ and density perturbation n_1 are nowhere divergent.

V. DISCUSSION

We have compared two hydrodynamic theories describing plasmon excitations in degenerate electron gases with one-dimensional spatial inhomogeneity. Their derivations differ principally by the way the pressure term is obtained.

The first theory, our HPT-N3 hydrodynamics, obtains the pressure term by identifying dispersive and compressive components, n_{1A} and n_{1B} , of the density perturbation n_1 : see Eqs. (7) - (10). n_{1A} is associated with the high-frequency pressure coefficient $\beta^2(\omega \rightarrow \infty) = \frac{3}{5}v_F^2$, while n_{1B} is associated with the low-pressure coefficient $\beta^2(\omega = 0) = \frac{1}{3}v_F^2$. See Eq. (11). (We will show elsewhere²⁶ that these associations arise naturally from a form of time-delayed scalar local density approximation for the pressure.) By these means we were able to satisfy the Harmonic Potential Theorem¹⁹ (HPT) and the usual conservation laws, and to obtain within the same formalism the correct plasmon dispersion of the uniform electron gas. The HPT applies to harmonically confined systems and constitutes a stringent test of an inhomogeneous many-particle theory, requiring in the present case that there exist a Kohn mode in which the inhomogeneous groundstate density profile $n_0(\vec{r})$ and pressure profile $P_0(\vec{r})$ move rigidly. This linear HPTN3 theory has been shown to give a sensible description²⁰ not only of the Kohn mode and other (standing) modes of harmonically confined systems, but also of multipole surface plasmons on a near-neutral jellium electron gas layer²⁶.

The second theory in our comparison is that of Tokatly and Pankratov²⁵ (TP). This was derived for degenerate systems by assuming the validity of a classical kinetic equation, then truncating the momentum moment equations. This yields a prediction for the pressure term. The truncation is justified, in the case of interest to us, by the smallness of the parameter $\gamma = v_F/(L\omega)$ where L and ω are the spatial scale and frequency. In order to compare with the HPT theory we needed to deal with inhomogeneous groundstates, and therefore we linearized the TP theory about the appropriate inhomogeneous Thomas-Fermi groundstate, a procedure not explicitly carried out by Tokatly and Pankratov.

Despite their quite different derivations, these two linearized theories give the same predictions for the case of one-dimensional spatial variation, as evidenced by the identity of Eqs. (14) and (31). This fact is the main result of the present paper.

The HPT-N3 derivation shows that the assumption of a classical kinetic equation, made by TP even in degenerate cases, is not necessary. On the other hand, the TP derivation is part of a systematic expansion whereas the HPT-N3 derivation is not obviously part of any

systematic scheme. Thus the two approaches are somewhat complementary, and each tends to support the validity of the other.

In order to be truly useful, the inhomogeneous formalisms discussed here should ideally be applicable at edges where the groundstate and/or excited electron density may vary rapidly in space. It is then likely that the TP truncation parameter γ (Eq. (17)) is small only at frequencies higher than the ones of interest. Nevertheless, in at least one important case covered by the Harmonic Potential Theorem, the formalism gives correct answers for very rapidly varying edge profiles. The use of these hydrodynamic approaches in regimes of rapid spatial variation is somewhat reminiscent of the commonplace and surprisingly successful use of the Local Density Functional formalism²⁷ for groundstate properties of highly inhomogeneous systems, despite the in-principle restriction to slow spatial variation. In that case the success is at least partly explained by the satisfaction of sum rules and constraints²⁸. The HPT constraint can be viewed in the same light for time-dependent cases, and indeed has already been used for this purpose in the context of the time-dependent Local Density Approximation for exchange and correlation²⁹. The connection of the present hydrodynamic approximations with finite-memory versions of density functional theory will be made more explicit elsewhere²⁶.

It should also be stressed that the existing HPT-N3 theory does not necessarily agree with the more general three-dimensional version¹⁵ of the TP theory. This is because the HPT-N3 theory to date has assumed a scalar pressure, whereas in the high-frequency plasmon case the pressure should certainly be a tensor, which indeed is what emerges from the 3D TP theory. It will be interesting to see if a tensor ansatz for the pressure, along the lines of the HPT-N3 argument, can re-derive the 3D TP theory.

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